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Molecular dynamics study of polymer-silica nanoparticle hybrids: Building blocks for directed assembly SABINA MASKEY, Clemson University, FLINT PIERCE, GARY GREST, Sandia National Laboratories, DVORA PERAHIA, Clemson University — Molecular dynamic simulations have been used to study the conformation and interactions of a polymer nanoparticle hybrid that consists of *para* dialkyl phenyleneethynylenes (PPEs) grafted to a silica nanoparticle, with the goal of deriving the factors that control their assembly. PPEs are electro-optically active polymers whose conformation determines their degree of conjugation and their assembly mode which in turn affects the electro-optical properties of the nanoparticle-polymer complexes. When confined to a nanoparticle surface, the PPE chains are fully extended in good solvents but cluster as the quality of the solvents is decreased. Tuning the degree of clustering by tuning the solvent-polymer interaction is expected to direct the assembly of the particles. Results for the conformation of grafted PPE molecules on a single nanoparticle and the forces between two nanoparticles as a function of solvent quality will be presented.

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